

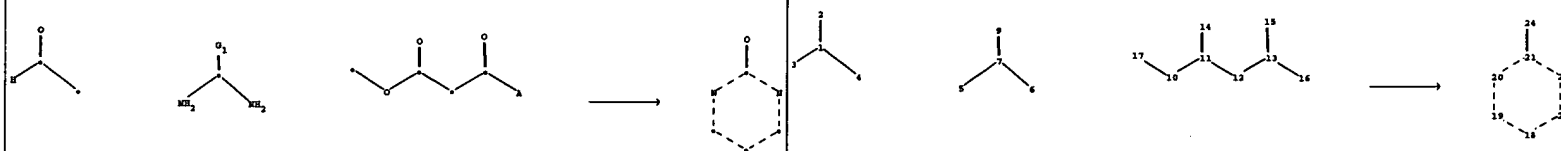
EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	1031	(544/315,318).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2006/06/25 14:42

NPL

		Results
5.	TITLE-ABSTR-KEY(polyaniline or poly aniline) and TITLE-ABSTR-KEY(pyrimidine) [All Sources(- All Sciences -)]	1
4.	TITLE-ABSTR-KEY(polyaniline or poly aniline) and TITLE-ABSTR-KEY (dihydropyrimidinone) [All Sources(- All Sciences -)]	0
3.	TITLE-ABSTR-KEY(polyaniline or poly aniline) [All Sources(- All Sciences -)]	3462
2.	TITLE-ABSTR-KEY(dihydropyrimidinone) and TITLE-ABSTR-KEY(polyaniline) [All Sources(- All Sciences -)]	0
1.	TITLE-ABSTR-KEY(dihydropyrimidinone) . [All Sources(- All Sciences -)]	73

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chain nodes :

1 2 3 5 6 7 9 10 11 12 13 14 15 24

ring nodes :

18 19 20 21 22 23

ring/chain nodes :

4 16 17

chain bonds :

1-2 1-3 1-4 5-7 6-7 7-9 10-11 10-17 11-12 11-14 12-13 13-15 13-16 21-24

ring bonds :

18-19 18-23 19-20 20-21 21-22 22-23

exact/norm bonds :

1-2 5-7 6-7 7-9 10-11 10-17 11-14 13-15 13-16 18-19 18-23 19-20 20-21 21-22
21-24 22-23

exact bonds :

1-3 1-4 11-12 12-13

isolated ring systems :

containing 18 :

G1:O,S

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS 10:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:CLASS

fragments assigned product role:

containing 18

fragments assigned reactant/reagent role:

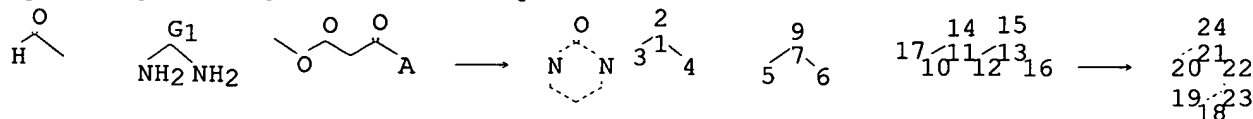
containing 1

containing 5

containing 10

=>

Uploading C:\Program Files\Stnexp\Queries\10810343.str



chain nodes :

1 2 3 5 6 7 9 10 11 12 13 14 15 24

ring nodes :

18 19 20 21 22 23

ring/chain nodes :

4 16 17

chain bonds :

1-2 1-3 1-4 5-7 6-7 7-9 10-11 10-17 11-12 11-14 12-13 13-15 13-16
21-24

ring bonds :

18-19 18-23 19-20 20-21 21-22 22-23

exact/norm bonds :

1-2 5-7 6-7 7-9 10-11 10-17 11-14 13-15 13-16 18-19 18-23 19-20 20-21
21-22 21-24 22-23

exact bonds :

1-3 1-4 11-12 12-13

isolated ring systems :

containing 18 :

G1:O,S

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS

fragments assigned product role:

containing 18

fragments assigned reactant/reagent role:

containing 1

containing 5

containing 10

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 13:24:00 FILE 'CASREACT'

SCREENING COMPLETE - 282 REACTIONS TO VERIFY FROM

23 DOCUMENTS

100.0% DONE 282 VERIFIED 95 HIT RXNS

6 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 4633 TO 6647

PROJECTED ANSWERS: 6 TO 266

L2 6 SEA SSS SAM L1 (95 REACTIONS)

=> => s l1 sss ful

FULL SEARCH INITIATED 13:26:41 FILE 'CASREACT'

SCREENING COMPLETE - 4674 REACTIONS TO VERIFY FROM

500 DOCUMENTS

100.0% DONE 4674 VERIFIED 2079 HIT RXNS

186 DOCS

SEARCH TIME: 00.00.01

L3 186 SEA SSS FUL L1 (2079 REACTIONS)

=> s polyanilin? or anilin?

67 POLYANILIN?

17462 ANILIN?

L4 17505 POLYANILIN? OR ANILIN?

=> s l3 and l4

L5 5 L3 AND L4

=> d l5 1-5 bib,ab,crdref

FAN.CNT 1

PRAI

AR

RX(1) OF 17



NOTE: optimization study

CON: 2 hours, 64 deg C

RX (2) OF 17

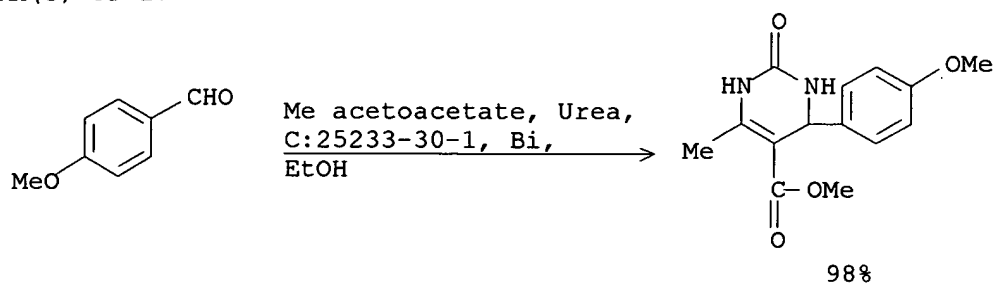


REF: U.S. Pat. Appl. Publ., 6 pp.; 2005

NOTE: catalyst is polyaniline-bismuth trichloride

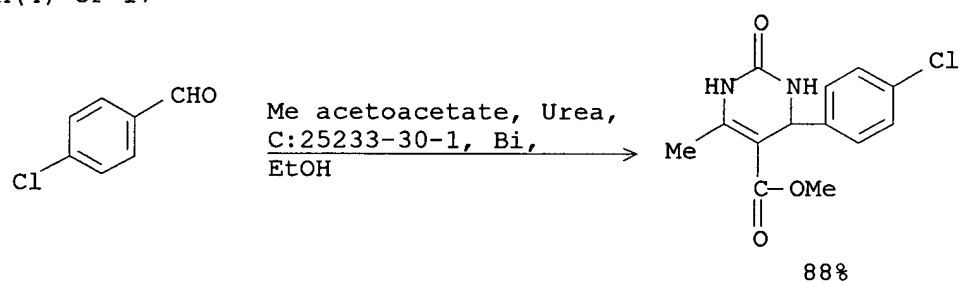
CON: 2 hours, reflux

RX(3) OF 17



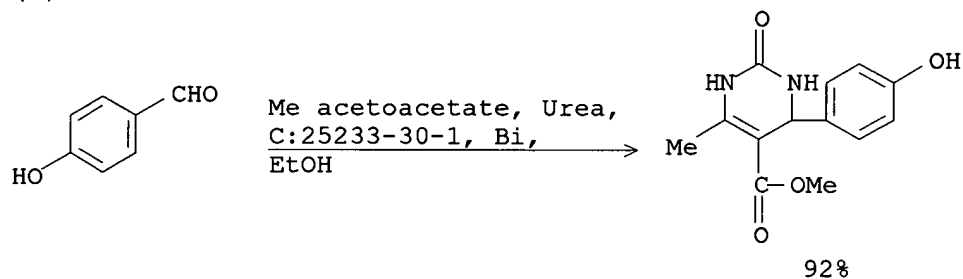
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 2 hours, reflux

RX(4) OF 17



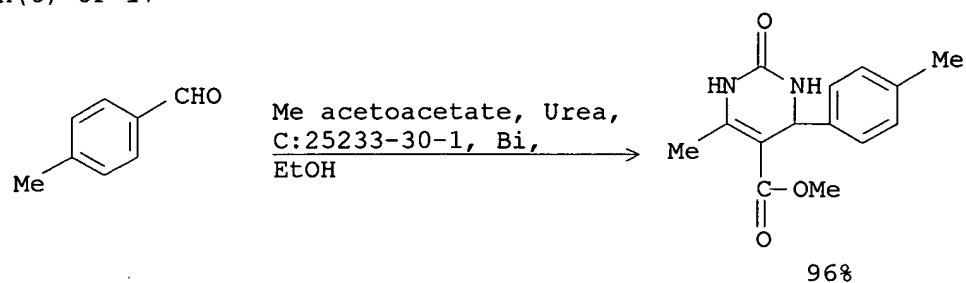
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 5 hours, reflux

RX(5) OF 17



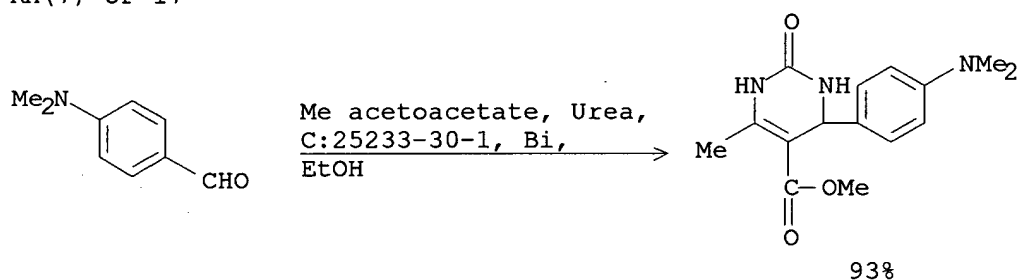
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 5 hours, reflux

RX(6) OF 17



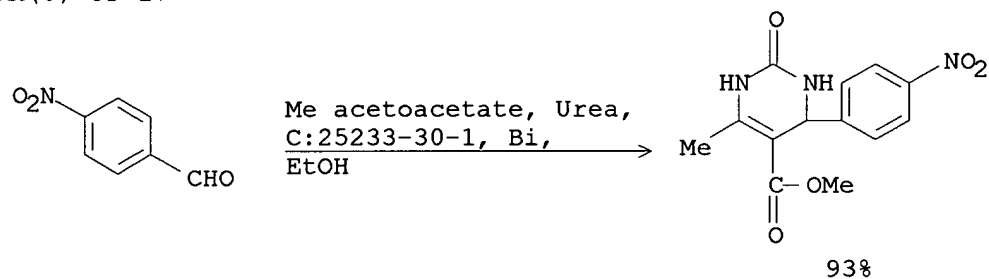
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 4 hours, reflux

RX(7) OF 17



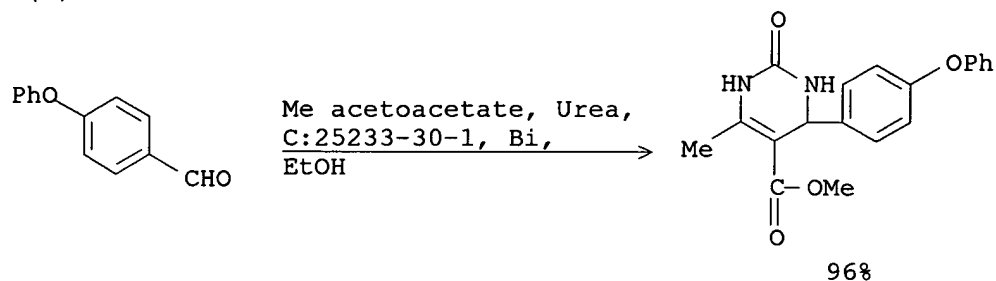
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 6 hours, reflux

RX(8) OF 17



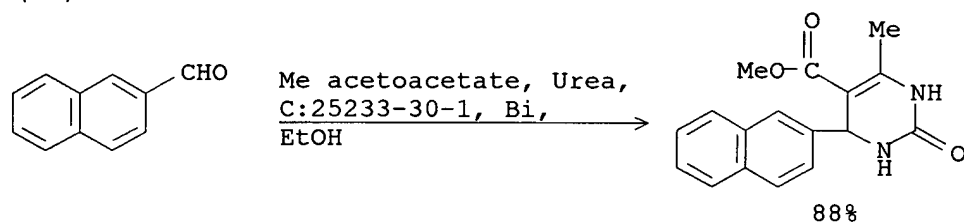
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 6 hours, reflux

RX(9) OF 17



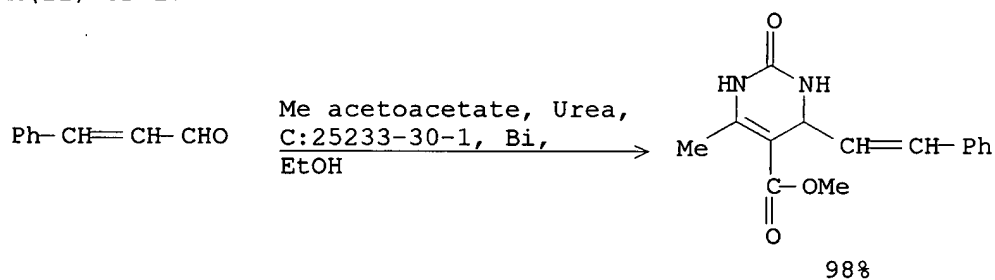
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 4 hours, reflux

RX(10) OF 17



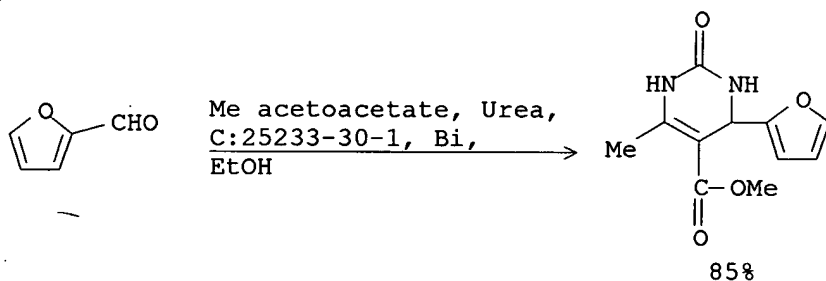
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 5 hours, reflux

RX(11) OF 17



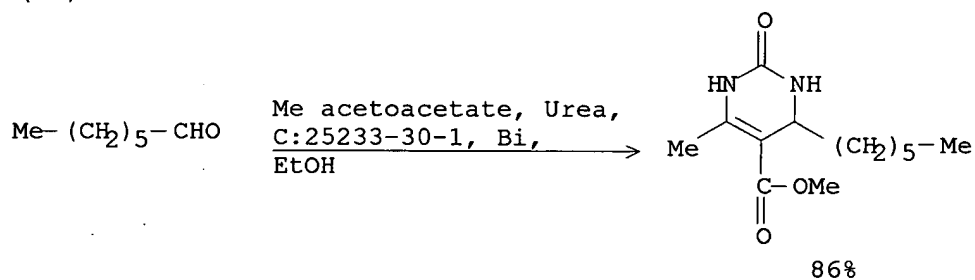
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 4 hours, reflux

RX(12) OF 17



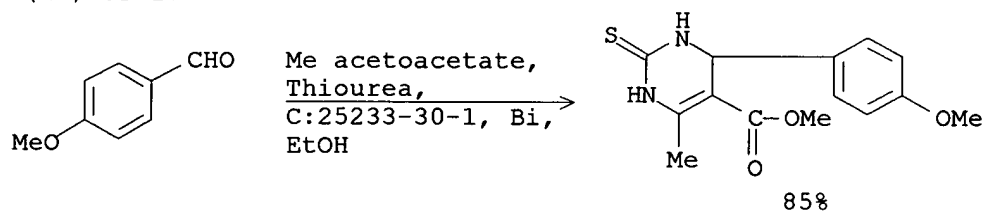
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 4 hours, reflux

RX(13) OF 17



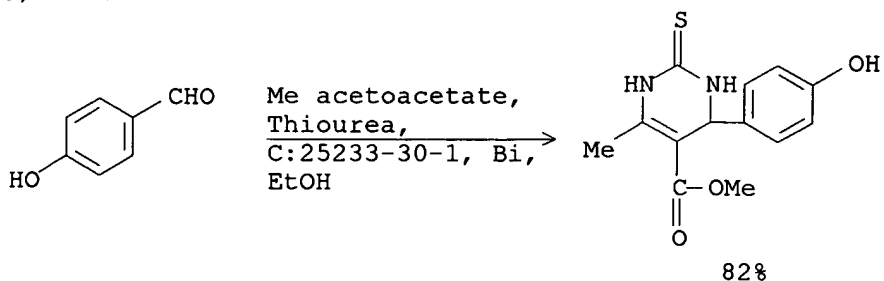
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 4 hours, reflux

RX(14) OF 17



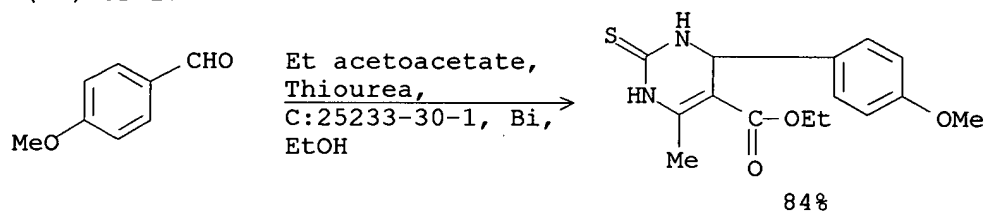
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 4 hours, reflux

RX(15) OF 17



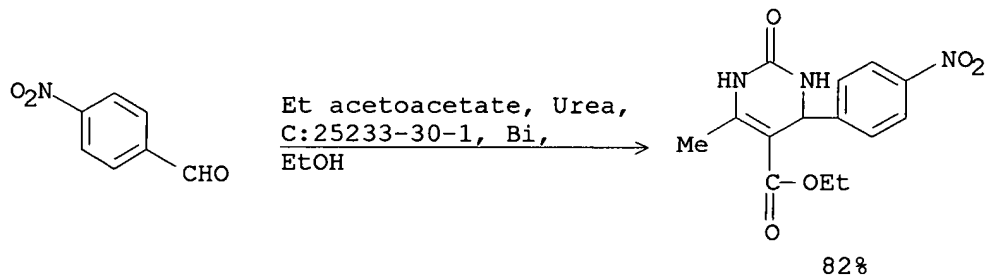
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 6 hours, reflux

RX(16) OF 17



REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 4 hours, reflux

RX(17) OF 17



REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
 NOTE: catalyst is polyaniline-bismuth trichloride
 CON: 6 hours, reflux

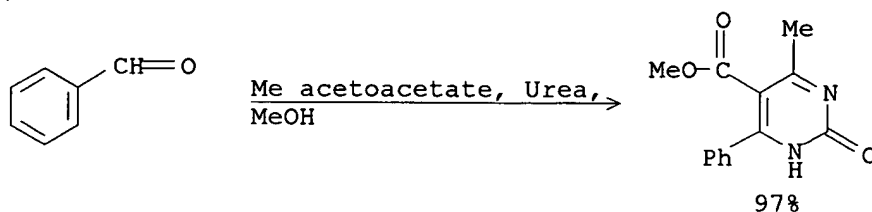
L5 ANSWER 2 OF 5 CASREACT COPYRIGHT 2006 ACS on STN
 AN 143:133385 CASREACT
 TI A preparation of dihydropyrimidinone derivatives from β -ketoester and (thio)urea in the presence of **polyaniline** salts
 IN Palaniappan, Srinivasan; Rao, Vaidya Jayathirtha; Banda, Gangadasu
 PA Council of Scientific & Industrial Research, India
 SO PCT Int. Appl., 12 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

Same Inv.
Appl
PCT

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005063719	A1	20050714	WO 2003-IN455	20031231
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003300711	A1	20050721	AU 2003-300711	20031231
PRAI WO 2003-IN455		20031231		

AB The invention relates to a preparation of dihydropyrimidinone derivs. from β -ketoester and (thio)urea in the presence of **polyaniline** salts as reusable catalysts. For instance, substituted dihydropyrimidinones were prepared via heterocyclization of urea, benzaldehyde, and Me acetoacetate in the presence of the prepared **polyaniline**-p-toluene sulfonate salt powder with a yield of 97% (reaction time: 120 min). A significant advantage of the invention is that the catalyst can be recycled to reaction mixture without significant loss in activity.

RX(1) OF 20

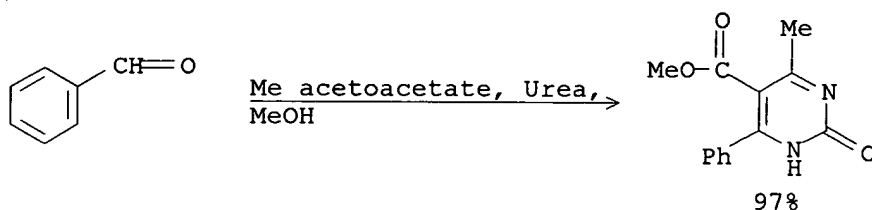


REF: PCT Int. Appl., 2005063719, 14 Jul 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 120 minutes, reflux

RX(2) OF 20

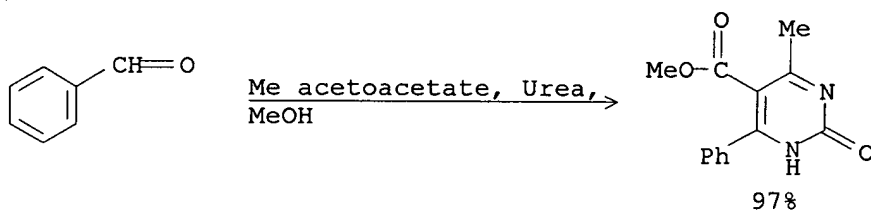


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 2 hours, 64 deg C

RX(3) OF 20

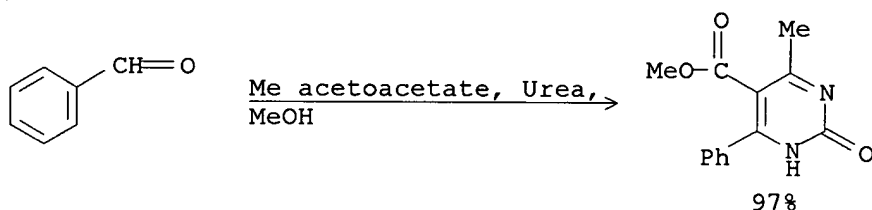


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 2 hours, reflux

RX(4) OF 20

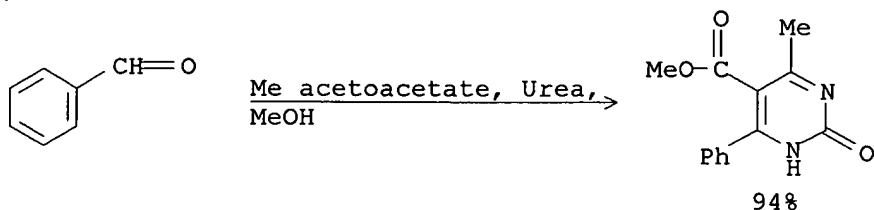


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 2 hours, reflux

RX(5) OF 20

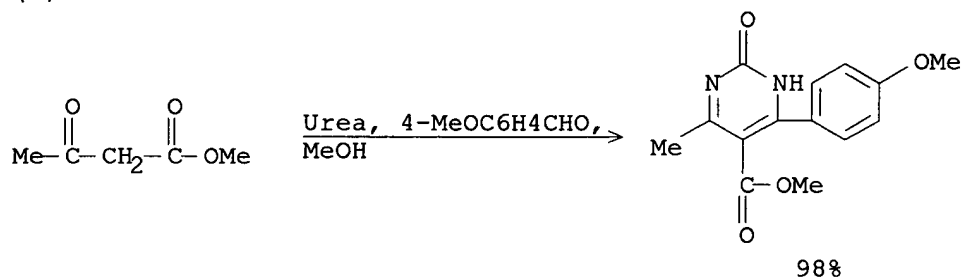


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 2 hours, reflux

RX(6) OF 20

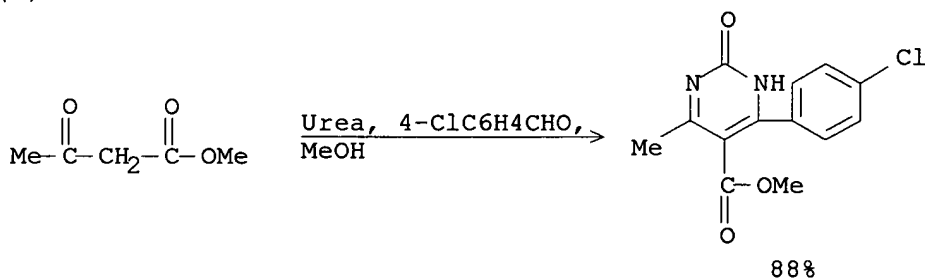


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 2 hours, reflux

RX(7) OF 20

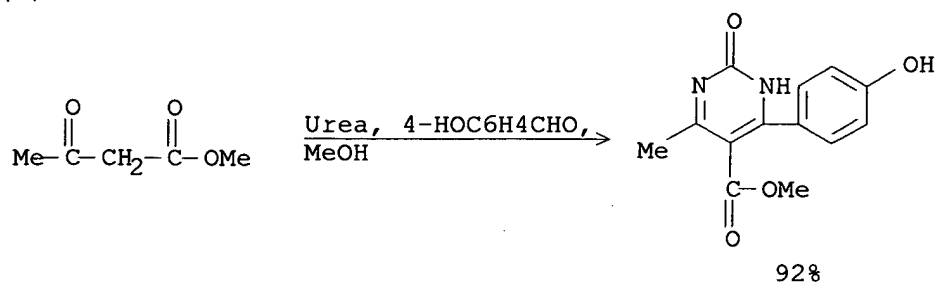


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 5 hours, reflux

RX(8) OF 20

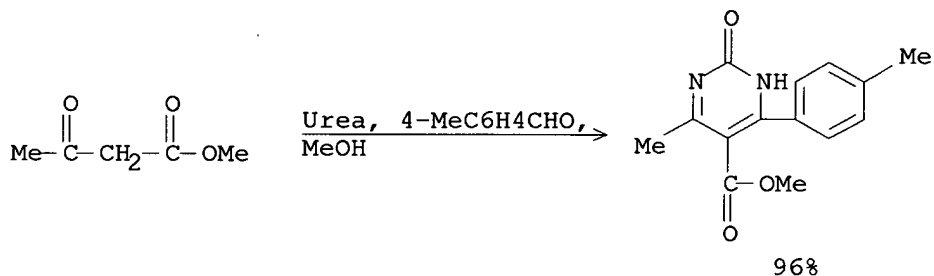


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 5 hours, reflux

RX(9) OF 20

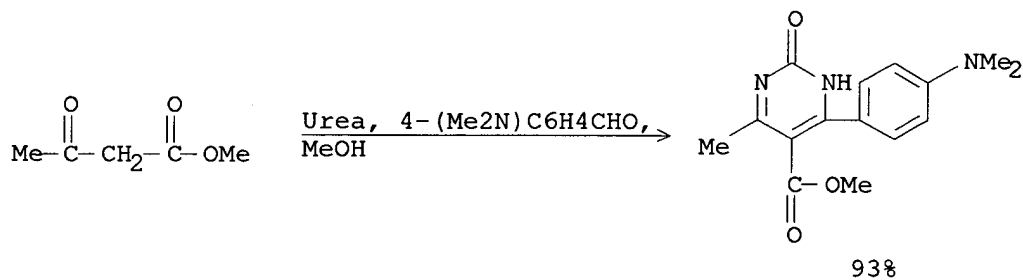


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 4 hours, reflux

RX(10) OF 20

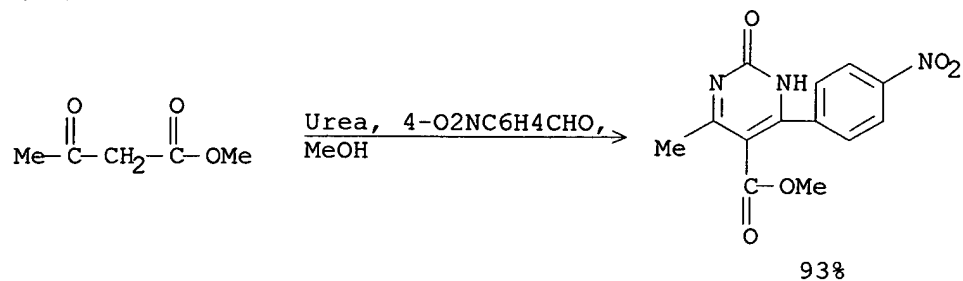


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 6 hours, reflux

RX(11) OF 20

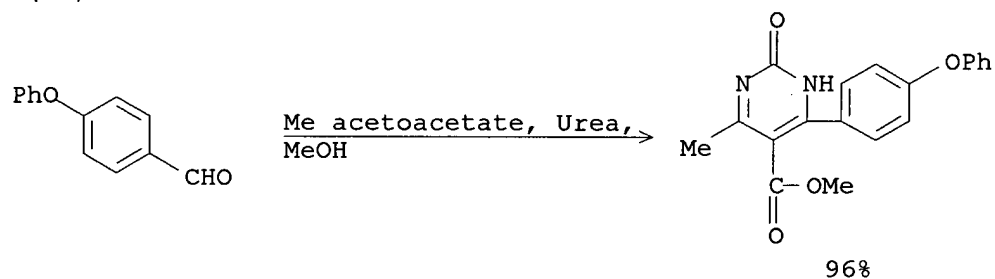


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 6 hours, reflux

RX(12) OF 20

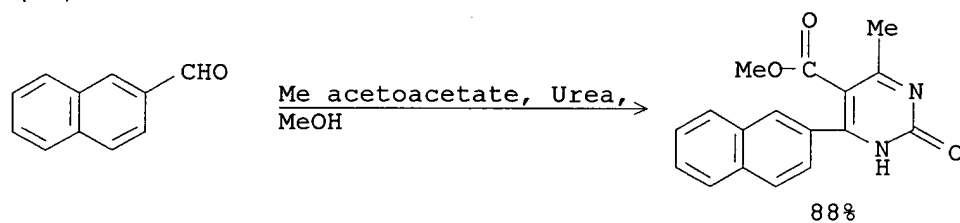


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 4 hours, reflux

RX(13) OF 20

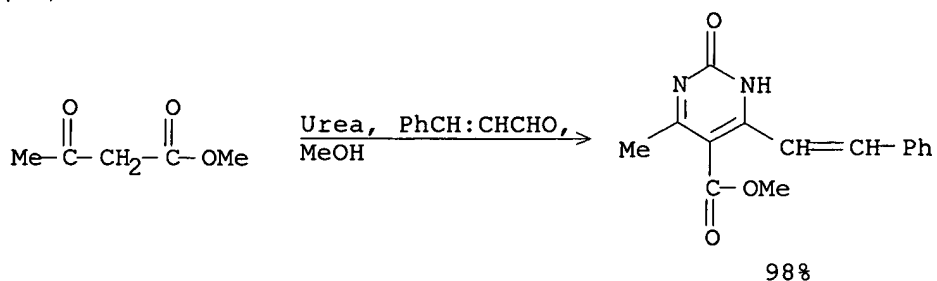


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 5 hours, reflux

RX(14) OF 20

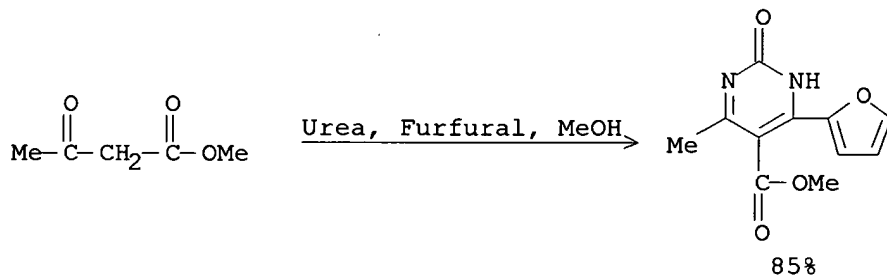


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 4 hours, reflux

RX(15) OF 20

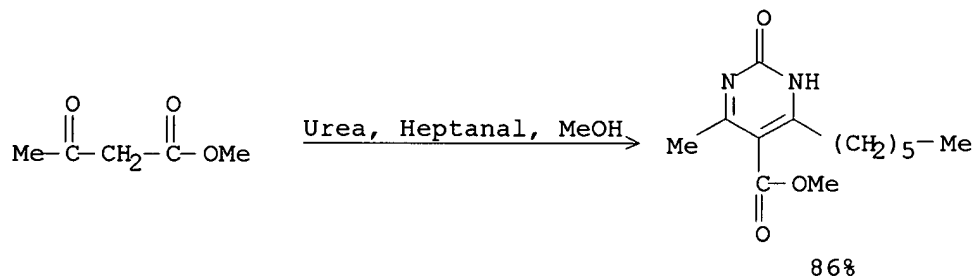


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 4 hours, reflux

RX(16) OF 20

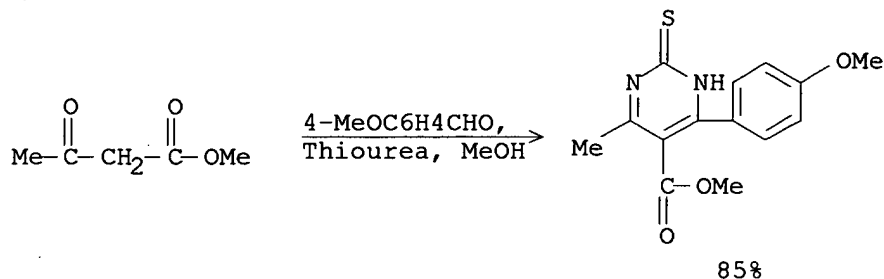


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 4 hours, reflux

RX(17) OF 20

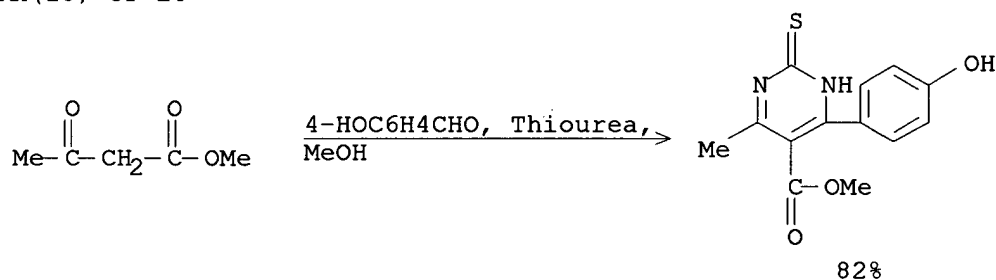


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 4 hours, reflux

RX(18) OF 20

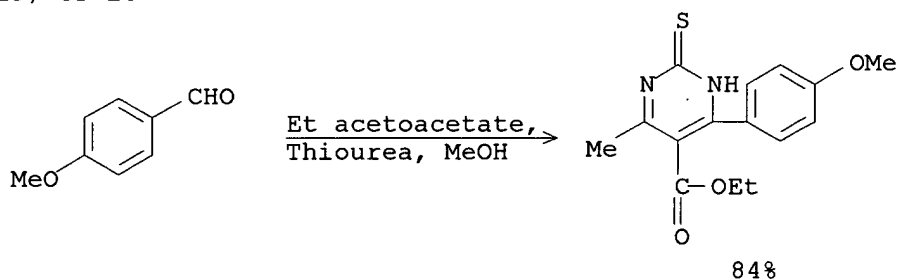


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 6 hours, reflux

RX(19) OF 20

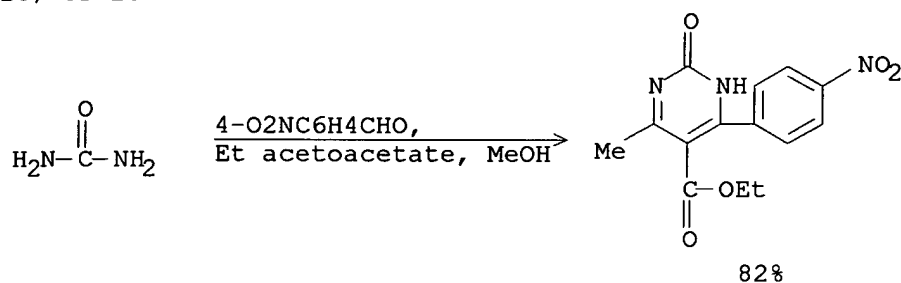


REF: PCT Int. Appl., 12 pp.; 2005

NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 4 hours, reflux

RX(20) OF 20



REF: PCT Int. Appl., 12 pp.; 2005

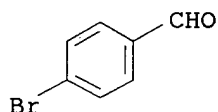
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst

CON: 6 hours, reflux

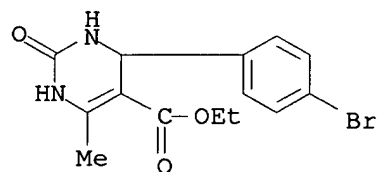
RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 5 CASREACT COPYRIGHT 2006 ACS on STN
 AN 143:26558 CASREACT
 TI Microwave-Enhanced and Metal-Catalyzed Functionalizations of the
 4-Aryl-Dihydropyrimidone Template
 AU Wannberg, Johan; Dallinger, Doris; Kappe, C. Oliver; Larhed, Mats
 CS Department of Medicinal Chemistry Organic, Pharmaceutical Chemistry, BMC,
 Uppsala University, Uppsala, Swed.
 SO Journal of Combinatorial Chemistry (2005), 7(4), 574-583
 CODEN: JCCHFF; ISSN: 1520-4766
 PB American Chemical Society
 DT Journal
 LA English
 AB Progress in organometallic catalysis and recent advancements in the
 development of carbonylative reaction protocols without direct use of
 carbon monoxide have been utilized for efficient functionalizations of
 4-aryldihydropyrimidone structures. The use of modern microwave technol.
 enabled both high reaction rates and convenient handling. Examples of
 palladium-catalyzed cross-couplings, Heck reactions, amino- and
 alkoxy-carbonylations, and direct N-amidations of 4-(bromophenyl)-
 dihydropyrimidones I (R1 = R2 = H; X = Br) with formation of I (R1 = R2 =
 H; X = MeO2C, MeCONH, BuNHCO, MeO2CCH=CH, Ph, PhCONH, PhCONHNHCO, etc.)
 were performed. Further, the first N3-arylations of the dihydropyrimidone
 ring system in I (R1 = H, Me; R2 = X = H) to give I (R1 = H, Me; R2 = Ph,
 3-MeOC6H4, 4-O2NC6H4, etc.; X = H) were successfully completed using the
 copper-catalyzed Goldberg reaction. Altogether, these protocols provide
 new tools for rapid generation of novel and diverse dihydropyrimidone
 derivs.

RX(1) OF 60



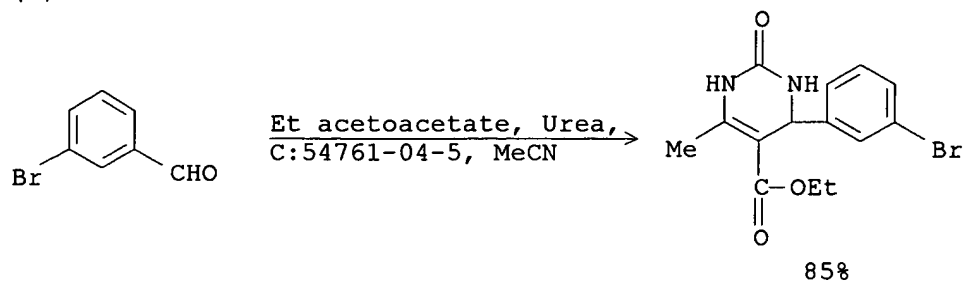
Et acetoacetate, Urea,
 C:54761-04-5, MeCN



77%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
 NOTE: microwave irradiation.
 CON: 15 minutes, 120 deg C

RX(2) OF 60

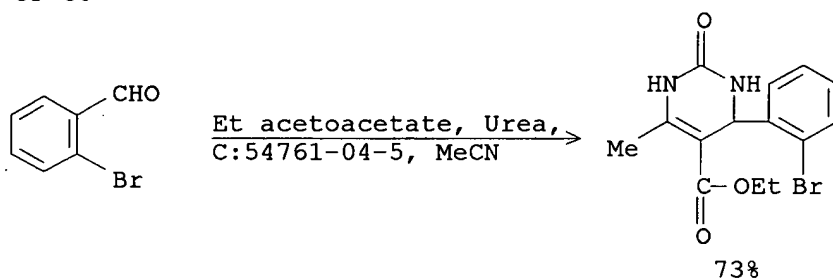


REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: microwave irradiation.

CON: 15 minutes, 120 deg C

RX(3) OF 60

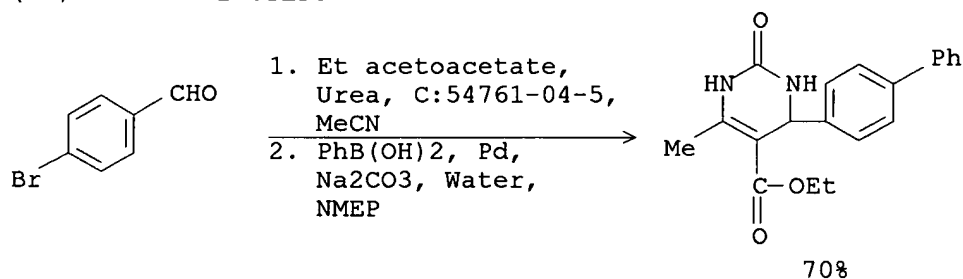


REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: microwave irradiation.

CON: 15 minutes, 120 deg C

RX(37) OF 60 - 2 STEPS



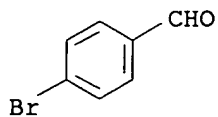
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

CON: STEP(1) 15 minutes, 120 deg C

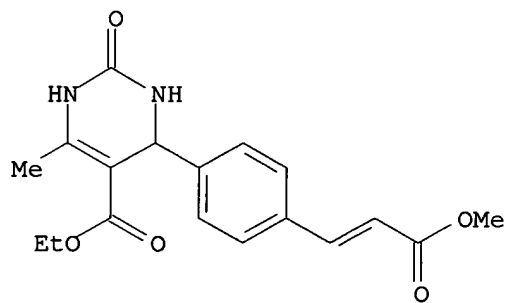
STEP(2) 20 minutes, 120 deg C

RX(38) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN

2.1. Pd(OAc)₂,
Tri-o-tolylphosphine,
EtN(Pr-i)₂, MeCN
2.2. Me acrylate



65%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

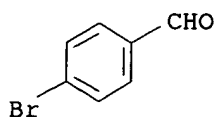
NOTE: 1) microwave irradiation, 2) microwave irradiation. second stage

CON: STEP(1) 15 minutes, 120 deg C

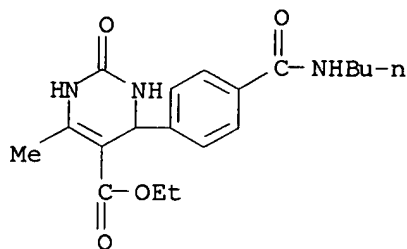
STEP(2.1) 45 minutes, 60 deg C

STEP(2.2) 30 minutes, 180 deg C

RX(39) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN
2. BuNH₂, Mo(CO)₆,
C:172418-32-5,
R:131274-22-1, DBU,
THF



87%

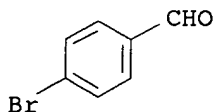
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

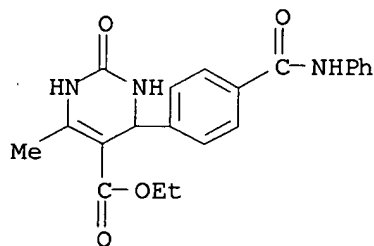
CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 130 deg C

RX(40) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN
2. PhNH₂, Mo(CO)₆,
C:172418-32-5,
R:131274-22-1, DBU,
THF



83%

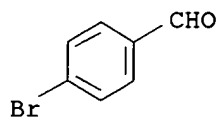
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

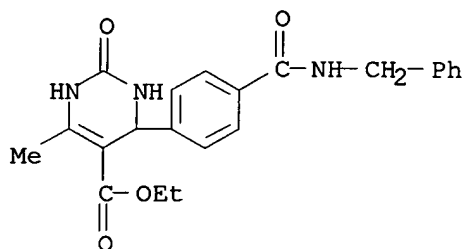
CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 130 deg C

RX(41) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN
2. PhCH₂NH₂, Mo(CO)₆,
C:172418-32-5,
R:131274-22-1, DBU,
THF



78%

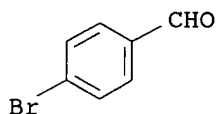
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

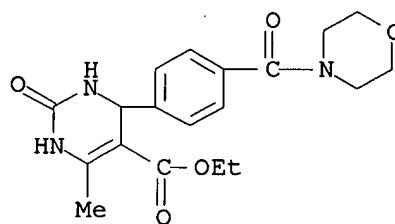
CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 130 deg C

RX(42) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN
2. Morpholine,
Mo(CO)₆,
C:172418-32-5,
R:131274-22-1, DBU,
THF



56%

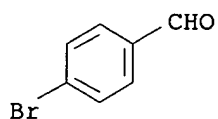
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

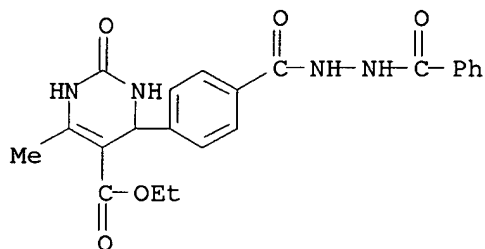
CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 140 deg C

RX(43) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN
2. BzNHNH2, Mo(CO)₆,
C:172418-32-5,
R:131274-22-1, DBU,
THF



35%

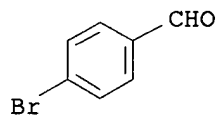
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

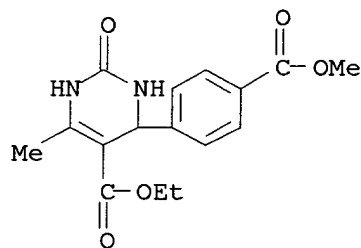
CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 5 minutes, 130 deg C

RX(44) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN
2. MeOH, Mo(CO)₆,
C:172418-32-5,
R:131274-22-1, DBU



77%

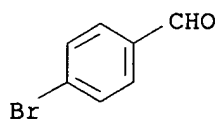
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

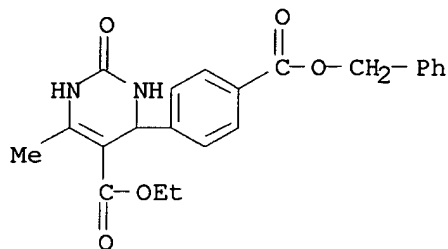
CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 110 deg C

RX(45) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN
2. PhCH₂OH, Mo(CO)₆,
C:172418-32-5,
R:131274-22-1, DBU,
THF



45%

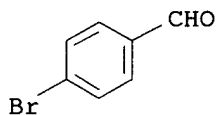
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

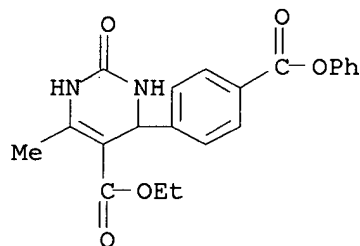
CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 140 deg C

RX(46) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN
2. PhOH, Mo(CO)₆,
C:172418-32-5,
R:131274-22-1, DBU,
THF



42%

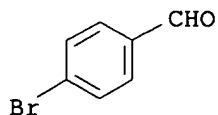
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

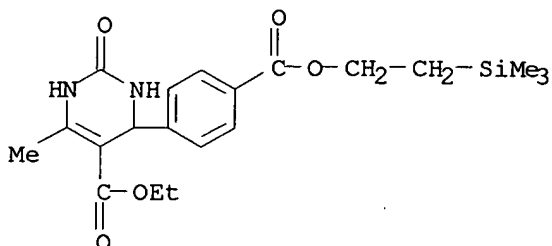
CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 140 deg C

RX(47) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN
2. $\text{Me}_3\text{SiCH}_2\text{CH}_2\text{OH}$,
 $\text{Mo}(\text{CO})_6$,
C:172418-32-5,
R:131274-22-1, DBU,
THF



52%

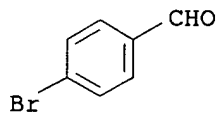
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

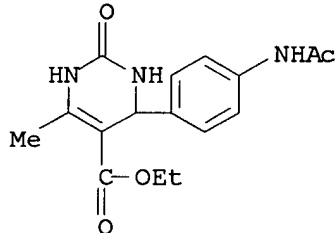
CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 140 deg C

RX(48) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN
2. AcNH_2 , $\text{Pd}(\text{OAc})_2$,
C:161265-03-8,
 Cs_2CO_3 , THF



85%

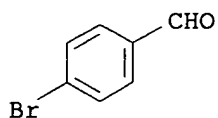
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

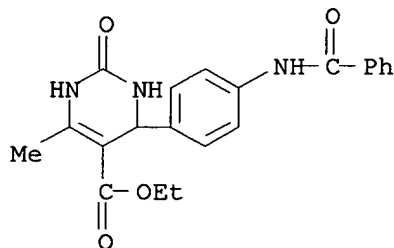
CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 140 deg C

RX(49) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN
2. BzNH₂, Pd(OAc)₂,
C:161265-03-8,
Cs₂CO₃, THF



72%

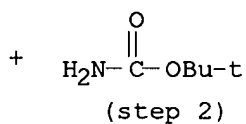
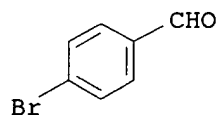
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

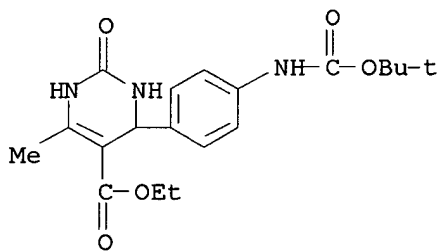
CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 120 deg C

RX(50) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN
2. Pd(OAc)₂,
C:161265-03-8,
Cs₂CO₃, THF



62%

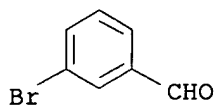
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

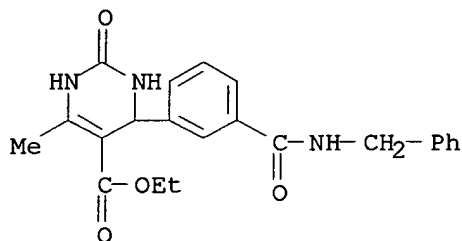
CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 150 deg C

RX(51) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN
2. PhCH₂NH₂, Mo(CO)₆,
C:172418-32-5,
R:131274-22-1, DBU,
THF



65%

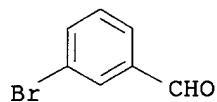
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

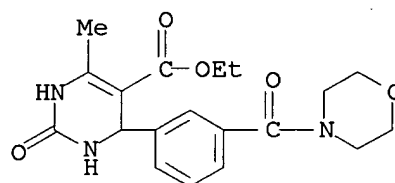
CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 130 deg C

RX(52) OF 60 - 2 STEPS



1. Et acetoacetate,
Urea, C:54761-04-5,
MeCN
2. Morpholine,
Mo(CO)₆,
C:172418-32-5,
R:131274-22-1, DBU,
THF



71%

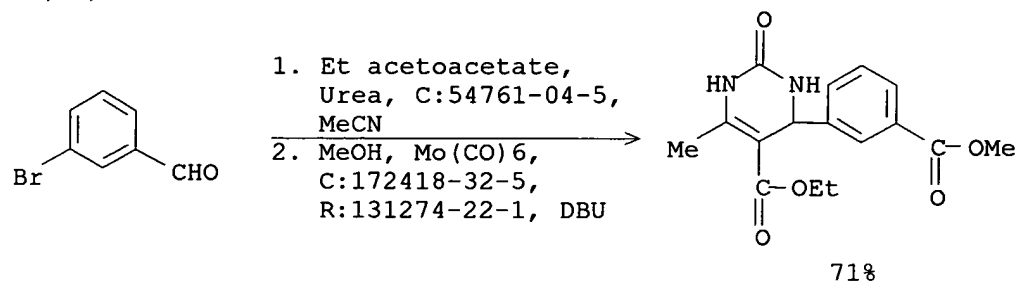
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 140 deg C

RX(53) OF 60 - 2 STEPS



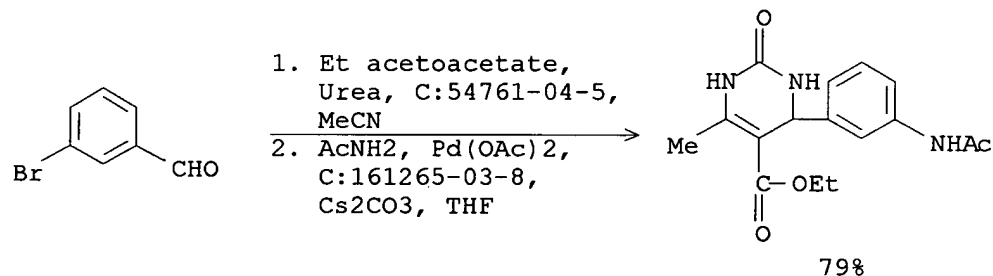
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 110 deg C

RX(54) OF 60 - 2 STEPS



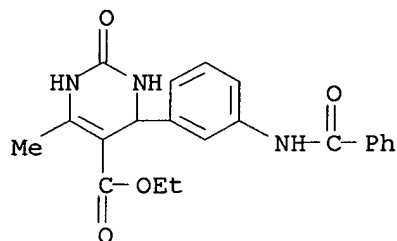
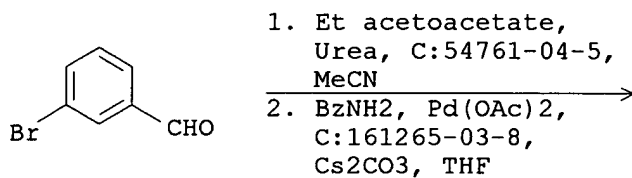
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 140 deg C

RX(55) OF 60 - 2 STEPS



88%

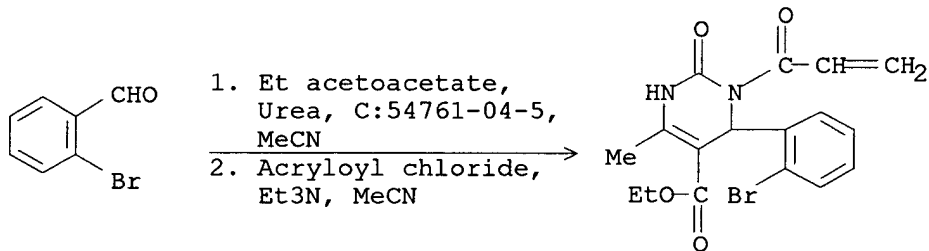
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 120 deg C

RX(56) OF 60 - 2 STEPS



62%

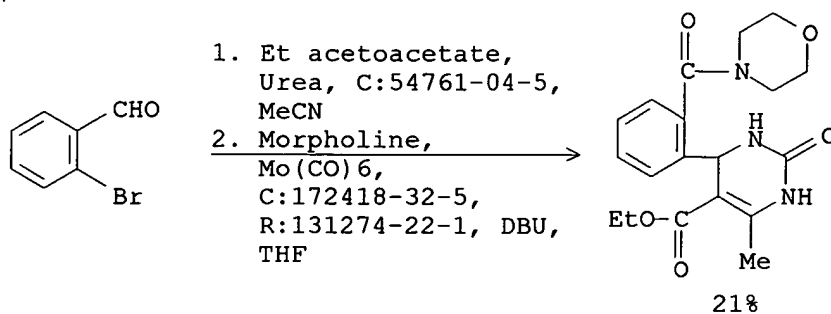
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation, regioselective

CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 20 minutes, 180 deg C

RX(57) OF 60 - 2 STEPS



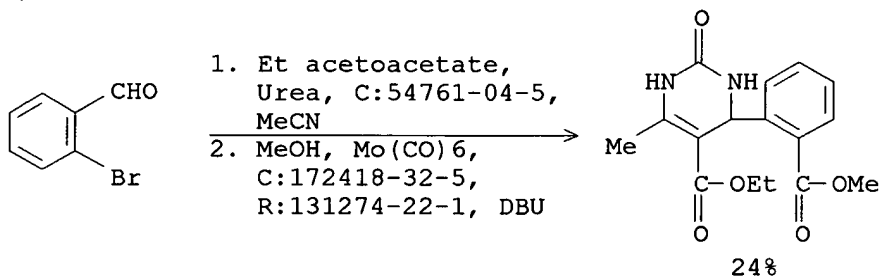
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 140 deg C

RX(58) OF 60 - 2 STEPS



REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradiation, 2) microwave irradiation.

CON: STEP(1) 15 minutes, 120 deg C

STEP(2) 15 minutes, 120 deg C

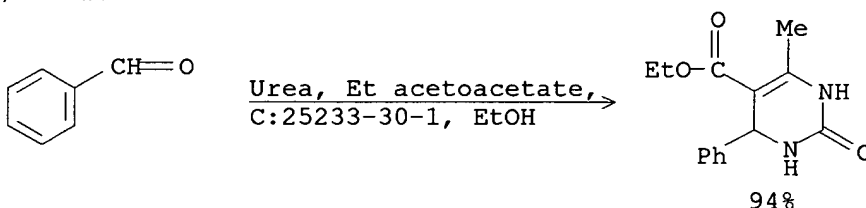
RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 5 CASREACT COPYRIGHT 2006 ACS on STN
 AN 141:207164 CASREACT
 TI One-pot synthesis of dihydropyrimidinones using **polyaniline**
 -bismoclite complex. A facile and reusable catalyst for the Biginelli
 reaction
 AU Gangadasu, Banda; Palaniappan, Srinivasan; Rao, Vaidya Jayathirtha
 CS Organic Chemistry Division II, Indian Institute of Chemical Technology,
 Hyderabad, 500 007, India
 SO Synlett (2004), (7), 1285-1287
 CODEN: SYNLES; ISSN: 0936-5214
 PB Georg Thieme Verlag
 DT Journal
 LA English
 AB **Polyaniline**-bismoclite complex was used as an efficient catalyst
 for the three-component condensation reaction of an aldehyde,
 β -ketoester, and urea in ethanol to afford the dihydropyrimidinones
 in excellent yields. Furthermore, after completion of reaction the
 catalyst could be easily recovered and reused without affecting its
 activity.

June, 2004

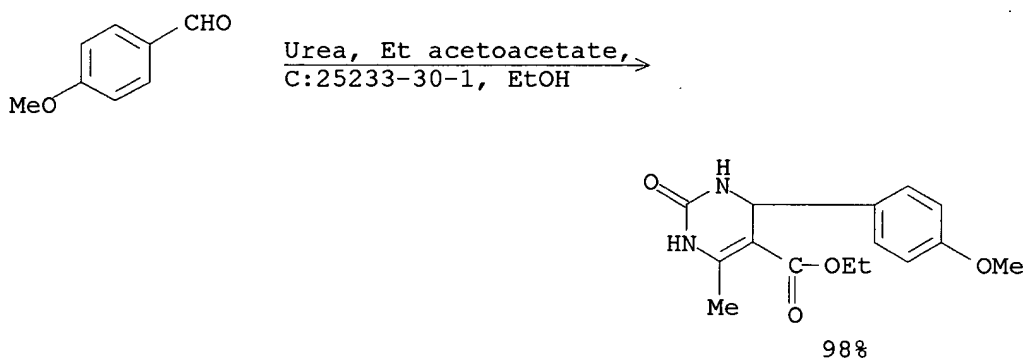
Not prior

RX(1) OF 14



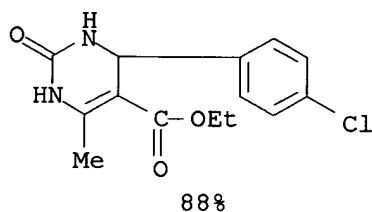
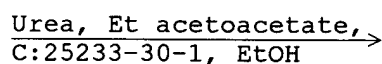
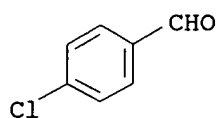
REF: Synlett, (7), 1285-1287; 2004
 NOTE: heated, Biginelli reaction
 CON: 2 hours

RX(2) OF 14



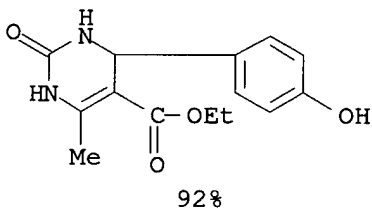
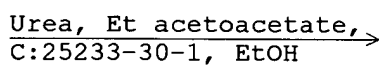
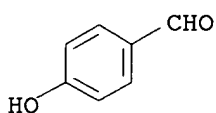
REF: Synlett, (7), 1285-1287; 2004
 NOTE: heated, Biginelli reaction
 CON: 2 hours

RX(3) OF 14



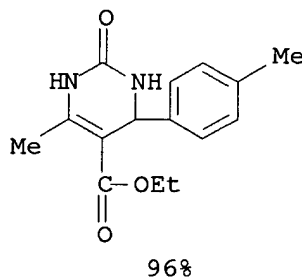
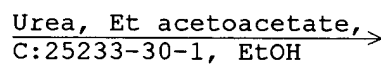
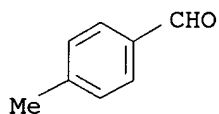
REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 5 hours

RX(4) OF 14



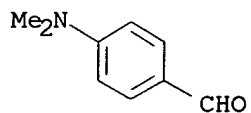
REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 5 hours

RX(5) OF 14

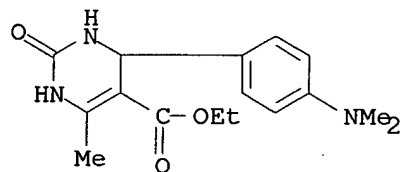


REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 4 hours

RX(6) OF 14



Urea, Et acetoacetate,
C:25233-30-1, EtOH



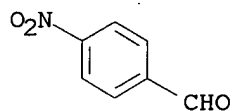
93%

REF: Synlett, (7), 1285-1287; 2004

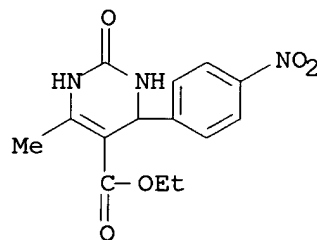
NOTE: heated, Biginelli reaction

CON: 6 hours

RX(7) OF 14



Urea, Et acetoacetate,
C:25233-30-1, EtOH



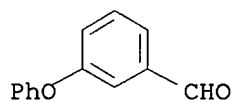
93%

REF: Synlett, (7), 1285-1287; 2004

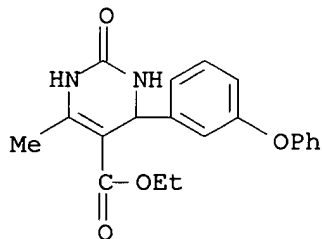
NOTE: heated, Biginelli reaction

CON: 6 hours

RX(8) OF 14



Urea, Et acetoacetate,
C:25233-30-1, EtOH



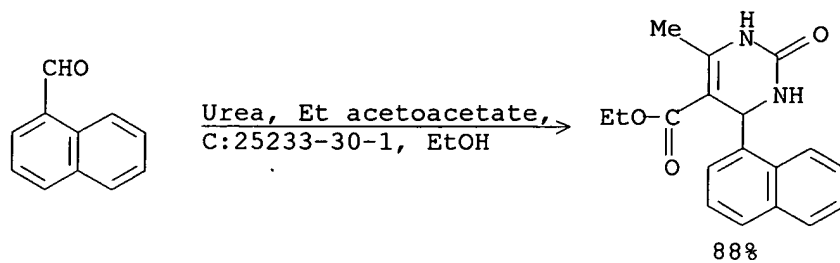
96%

REF: Synlett, (7), 1285-1287; 2004

NOTE: heated, Biginelli reaction

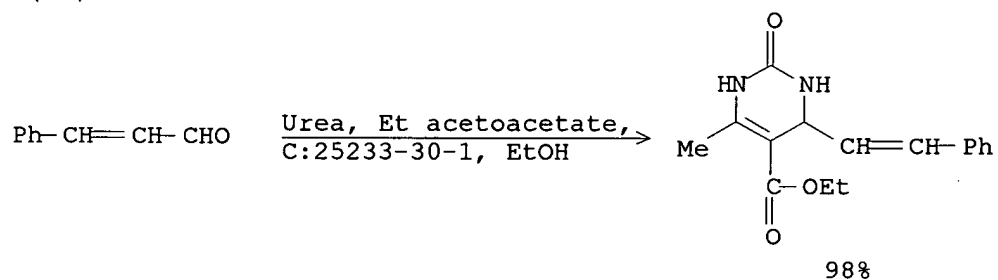
CON: 4 hours

RX(9) OF 14



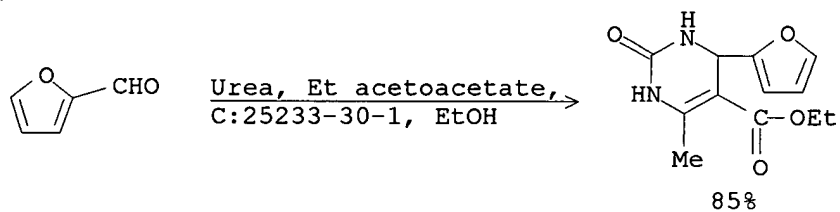
REF: Synlett, (7), 1285-1287; 2004
 NOTE: heated, Biginelli reaction
 CON: 5 hours

RX(10) OF 14



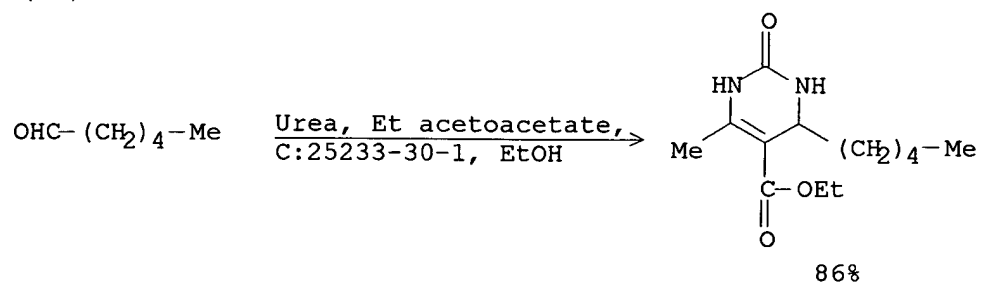
REF: Synlett, (7), 1285-1287; 2004
 NOTE: heated, Biginelli reaction
 CON: 4 hours

RX(11) OF 14



REF: Synlett, (7), 1285-1287; 2004
 NOTE: heated, Biginelli reaction
 CON: 4 hours

RX(12) OF 14



REF: Synlett, (7), 1285-1287; 2004

NOTE: heated, Biginelli reaction

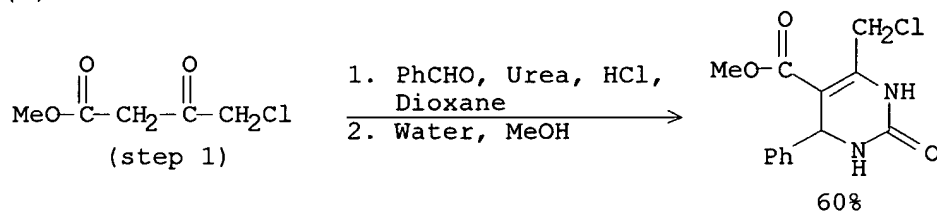
CON: 4 hours

RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 5 CASREACT COPYRIGHT 2006 ACS on STN
 AN 137:232612 CASREACT
 TI Traceless Solid-Phase Synthesis of Bicyclic Dihydropyrimidones Using
 Multidirectional Cyclization Cleavage
 AU Perez, Rolando; Beryozkina, Tetyana; Zbruyev, Oleksandr I.; Haas, Wilhelm;
 Kappe, C. Oliver
 CS Institute of Chemistry, Karl-Franzens-University Graz, Graz, A-8010,
 Austria
 SO Journal of Combinatorial Chemistry (2002), 4(5), 501-510
 CODEN: JCCHFF; ISSN: 1520-4766
 PB American Chemical Society
 DT Journal
 LA English
 AB Furopyrimidinediones I [R = Ph, 4-MeC₆H₄, 2-ClC₆H₄, 3-O₂NC₆H₄, 4-FC₆H₄,
 2,3-Cl₂C₆H₃, 3,4-F₂C₆H₃, 2-naphthyl, 2-F₃CC₆H₄, 4-BrC₆H₄, 3,4-(MeO)₂C₆H₃,
 2-thienyl], pyrrolopyrimidinediones II [R = Ph, 4-MeC₆H₄, 2-ClC₆H₄,
 3-O₂NC₆H₄, 4-FC₆H₄, 3,4-F₂C₆H₃, 2-naphthyl, 4-BrC₆H₄, 3,4-(MeO)₂C₆H₃,
 2-thienyl; R₁ = EtCH₂, Me₂CHCH₂CH₂, HOCH₂CH₂, H₂C:CHCH₂, c-C₆H₁₁, Ph,
 PhCH₂, 3-MeC₆H₄CH₂, 2-ClC₆H₄CH₂, 2-MeOC₆H₄CH₂CH₂, 4-FC₆H₄CH₂CH₂], and
 pyrimidopyridazinediones III [R = Ph, 4-MeC₆H₄, 2-ClC₆H₄, 4-FC₆H₄,
 3,4-F₂C₆H₃, 4-BrC₆H₄, 3,4-(MeO)₂C₆H₃, 2-thienyl; R₂ = H, Me, Ph] were
 prepared by solid- and solution-phase synthetic procedures using the Biginelli
 condensation reaction as the key steps. Condensation of aromatic aldehydes,
 and urea neat in the presence of HCl yielded the intermediate chloromethyl
 oxodihydropyrimidinecarboxylates IV [R = Ph, 4-MeC₆H₄, 2-ClC₆H₄,
 3-O₂NC₆H₄, 4-FC₆H₄, 2,3-Cl₂C₆H₃, 3,4-F₂C₆H₃, 2-naphthyl] in 27-72% yields;
 heating IV neat at 210° yielded I [R = Ph, 4-MeC₆H₄, 2-ClC₆H₄,
 3-O₂NC₆H₄, 4-FC₆H₄, 2,3-Cl₂C₆H₃, 3,4-F₂C₆H₃, 2-naphthyl] in 58-72% yields.
 Treatment of IV [R = Ph, 4-MeC₆H₄, 2-ClC₆H₄, 3-O₂NC₆H₄, 4-FC₆H₄,
 2,3-Cl₂C₆H₃, 3,4-F₂C₆H₃, 2-naphthyl] with amines in MeOH provided II [R =
 Ph, 4-MeC₆H₄, 2-ClC₆H₄, 3-O₂NC₆H₄, 4-FC₆H₄, 2,3-Cl₂C₆H₃, 3,4-F₂C₆H₃,
 2-naphthyl; R₁ = EtCH₂, HOCH₂CH₂, H₂C:CHCH₂, c-C₆H₁₁, PhCH₂, 3-MeC₆H₄CH₂,
 2-ClC₆H₄CH₂, 2-MeOC₆H₄CH₂CH₂, 4-FC₆H₄CH₂CH₂] in 33-74% yields; treatment
 of IV with hydrazines in dioxane or EtOH yielded III [R = Ph, 4-MeC₆H₄,
 2-ClC₆H₄, 4-FC₆H₄, 3,4-F₂C₆H₃; R₂ = H, Me, Ph] in 26-82% yields. The
 solid-phase sequence involves the initial high-speed, microwave-promoted
 acetoacetylation of hydroxymethylpolystyrene resin with Me
 4-chloroacetoacetate to give a resin-bound chloroacetoacetate ester;
 three-component Biginelli-type condensations with urea and aromatic aldehydes
 yielded resin-bound chloromethyl oxodihydropyrimidinecarboxylates.
 Microwave flash heating of resin-bound chloromethyl
 oxodihydropyrimidinecarboxylates for 10 min at 150° yielded I [R =
 Ph, 4-MeC₆H₄, 2-ClC₆H₄, 3-O₂NC₆H₄, 4-FC₆H₄, 2,3-Cl₂C₆H₃, 3,4-F₂C₆H₃,
 2-naphthyl, 2-F₃CC₆H₄, 4-BrC₆H₄, 3,4-(MeO)₂C₆H₃, 2-thienyl] in 14-77%
 yields. Addition of amines to the resin-bound chloromethyl
 oxodihydropyrimidinecarboxylate intermediates at either ambient temperature or
 at 50° gave aminomethyl oxodihydropyrimidinecarboxylates which
 underwent cyclization and resin cleavage by microwave irradiation at
 150-250° for 10 min. to give II [R = Ph, 4-MeC₆H₄, 2-ClC₆H₄,
 3-O₂NC₆H₄, 4-FC₆H₄, 3,4-F₂C₆H₃, 2-naphthyl, 4-BrC₆H₄, 3,4-(MeO)₂C₆H₃,
 2-thienyl; R₁ = EtCH₂, Me₂CHCH₂CH₂, HOCH₂CH₂, H₂C:CHCH₂, c-C₆H₁₁, Ph,
 PhCH₂, 3-MeC₆H₄CH₂, 2-ClC₆H₄, 2-MeOC₆H₄CH₂CH₂, 4-FC₆H₄CH₂CH₂] in 15-55%
 yields. Addition of hydrazines to the resin-bound chloromethyl
 oxodihydropyrimidinecarboxylate intermediates at either ambient temperature
 gave
 hydrazinomethyl oxodihydropyrimidinecarboxylates which underwent
 cyclization and resin cleavage by microwave irradiation at 150° for 10
 min. to give III [R = Ph, 2-ClC₆H₄, 3,4-F₂C₆H₃, 4-BrC₆H₄, 3,4-(MeO)₂C₆H₃,

2-thienyl; R2 = H, Me] in 30-41% yields. Resin cleavage in the solid-phase syntheses was traceless and did not involve addnl. steps in the preparation of the target compds.

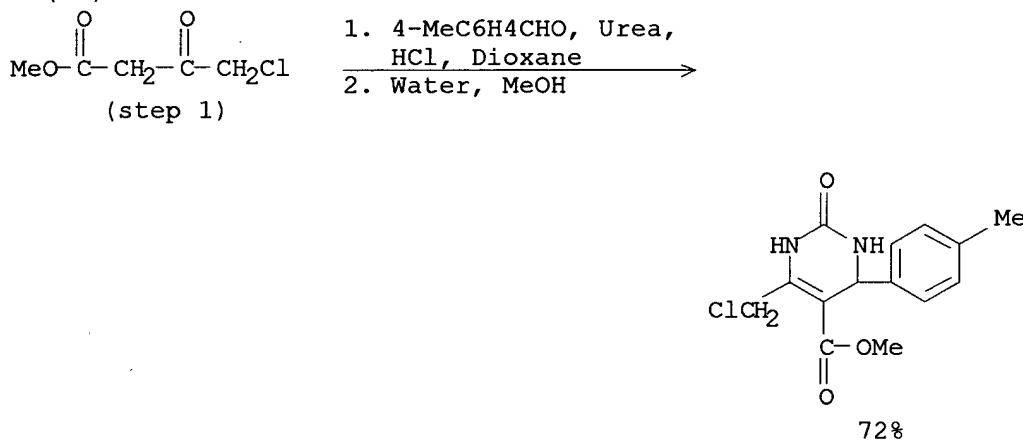
RX(9) OF 108



REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002

NOTE: KEY STEP, Biginelli condensation

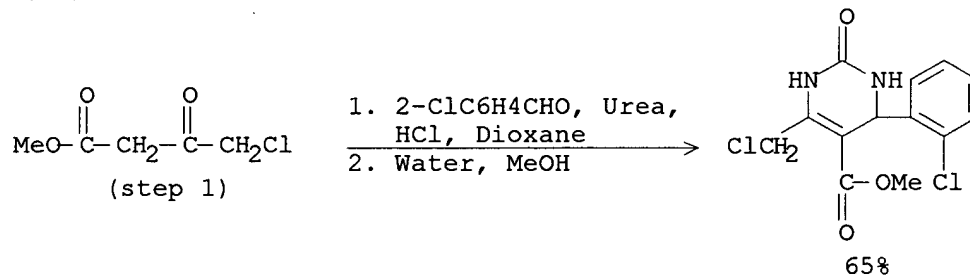
RX(10) OF 108



REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002

NOTE: KEY STEP, Biginelli condensation

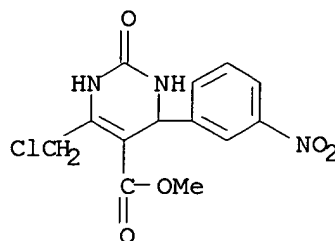
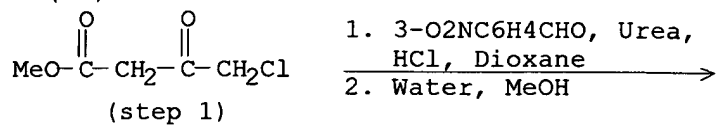
RX(11) OF 108



REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002

NOTE: KEY STEP, Biginelli condensation

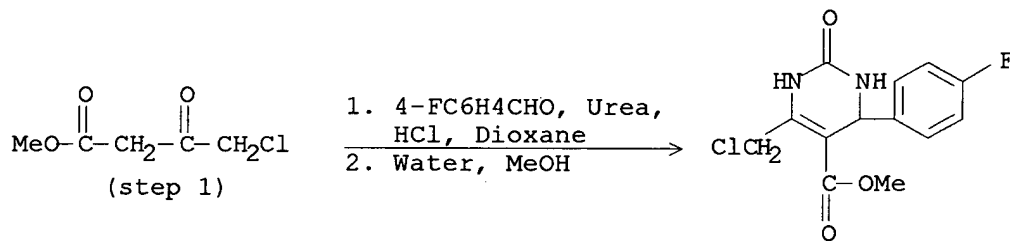
RX(12) OF 108



27%

REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
 NOTE: KEY STEP, Biginelli condensation

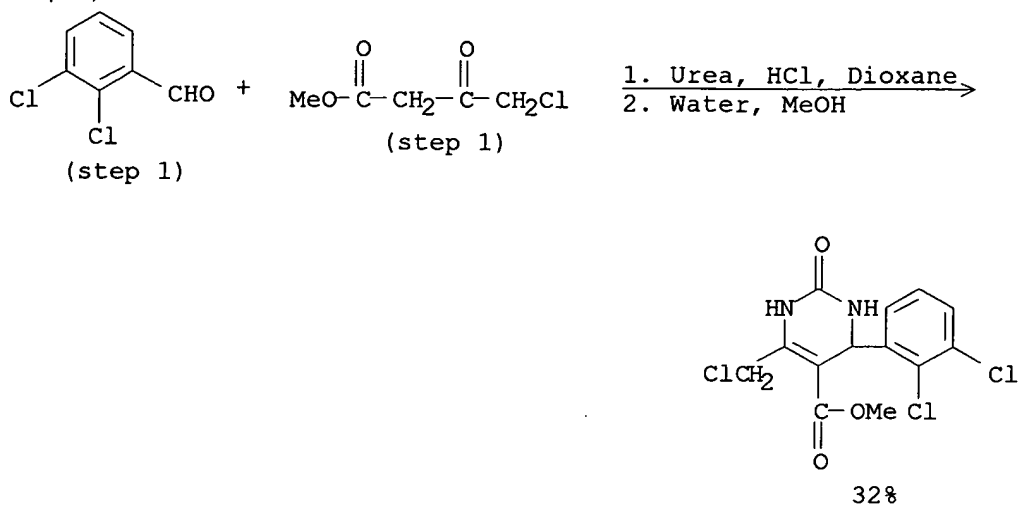
RX(13) OF 108



68%

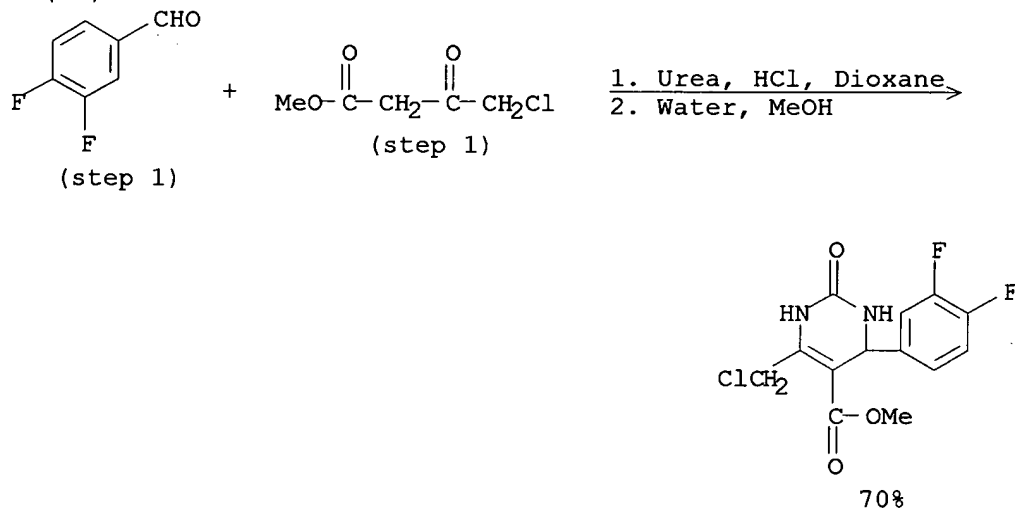
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 NOTE: KEY STEP, Biginelli condensation

RX(14) OF 108



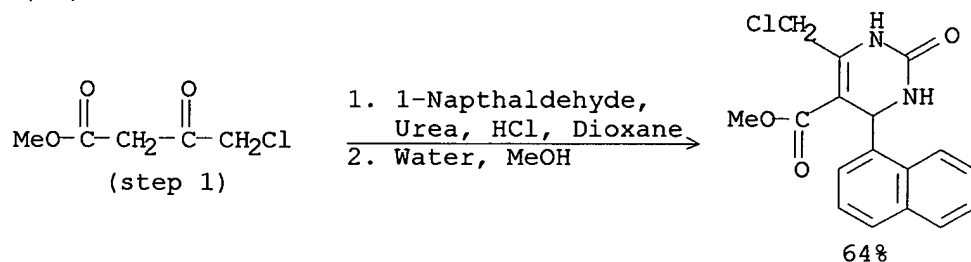
REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
NOTE: KEY STEP, Biginelli condensation

RX(15) OF 108



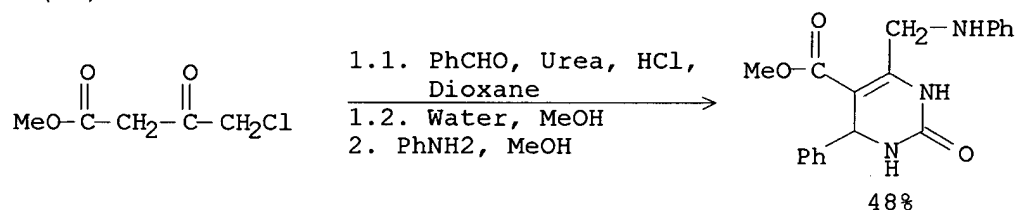
REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
NOTE: KEY STEP, Biginelli condensation

RX(16) OF 108



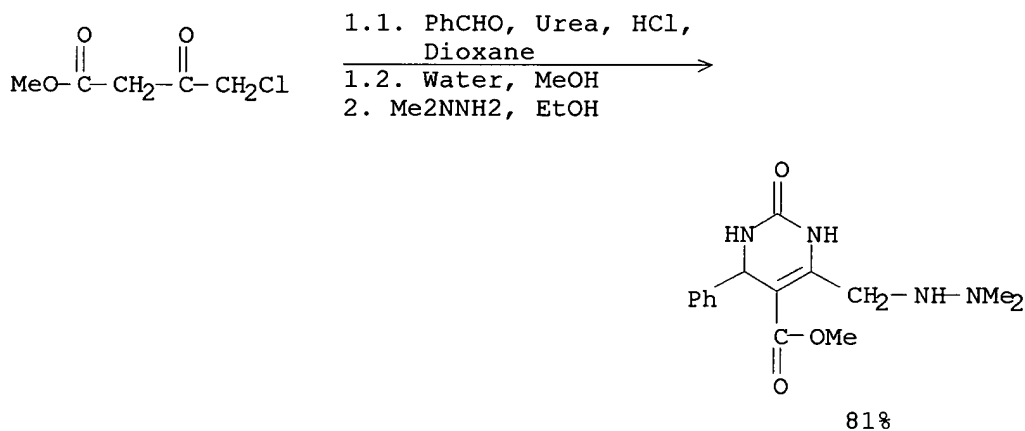
REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
 NOTE: KEY STEP, Biginelli condensation

RX(84) OF 108 - 2 STEPS



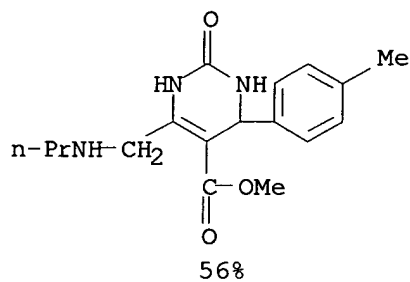
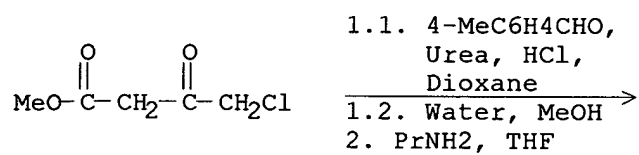
REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
 NOTE: 1) KEY STEP, Biginelli condensation

RX(86) OF 108 - 2 STEPS



REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
 NOTE: 1) KEY STEP, Biginelli condensation

RX(91) OF 108 - 2 STEPS



REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
 NOTE: 1) KEY STEP, Biginelli condensation

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 ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.30

146.29

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

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